



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:35 am BST

PDB ID : 1Y11  
Title : Mycobacterial adenylyl cyclase Rv1264, holoenzyme, active state  
Authors : Tews, I.; Findeisen, F.; Sinning, I.; Schultz, A.; Schultz, J.E.; Linder, J.U.  
Deposited on : 2004-11-16  
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

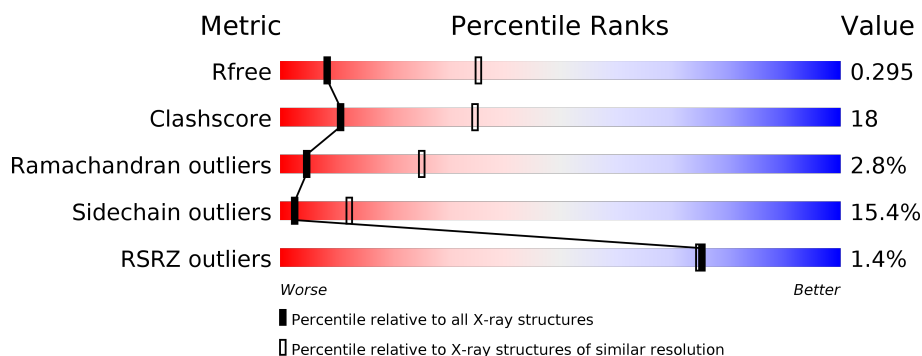
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	407	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2764 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hypothetical protein Rv1264/MT1302.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2737	1716	501	509	11			

There are 10 discrepancies between the modelled and reference sequences:

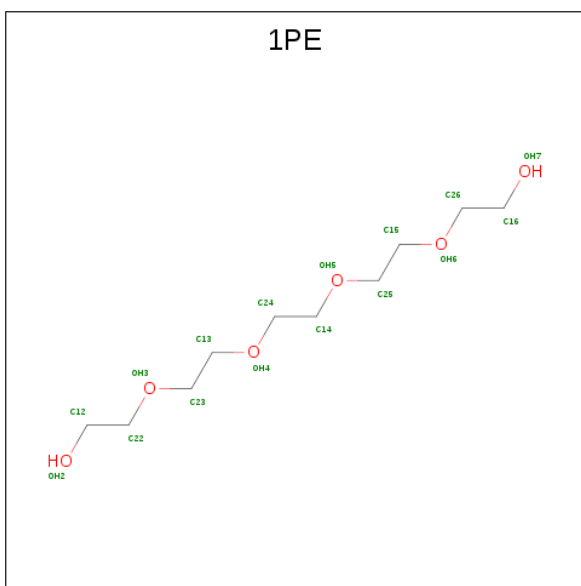
Chain	Residue	Modelled	Actual	Comment	Reference
A	398	GLY	-	EXPRESSION TAG	UNP Q11055
A	399	SER	-	EXPRESSION TAG	UNP Q11055
A	400	ARG	-	EXPRESSION TAG	UNP Q11055
A	401	SER	-	EXPRESSION TAG	UNP Q11055
A	402	HIS	-	EXPRESSION TAG	UNP Q11055
A	403	HIS	-	EXPRESSION TAG	UNP Q11055
A	404	HIS	-	EXPRESSION TAG	UNP Q11055
A	405	HIS	-	EXPRESSION TAG	UNP Q11055
A	406	HIS	-	EXPRESSION TAG	UNP Q11055
A	407	HIS	-	EXPRESSION TAG	UNP Q11055

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



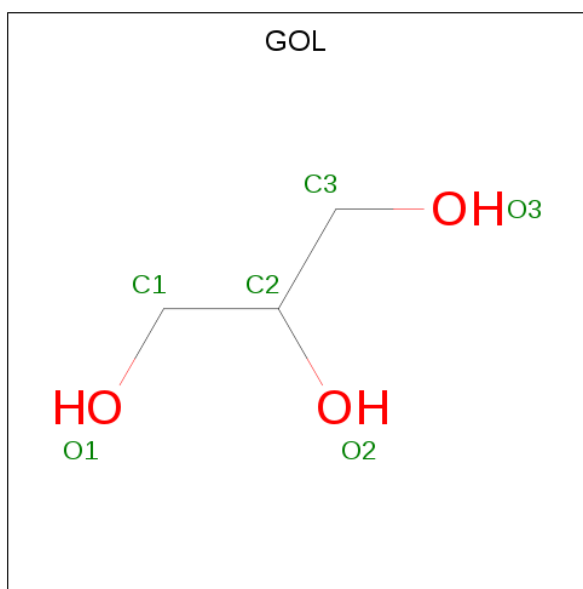
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

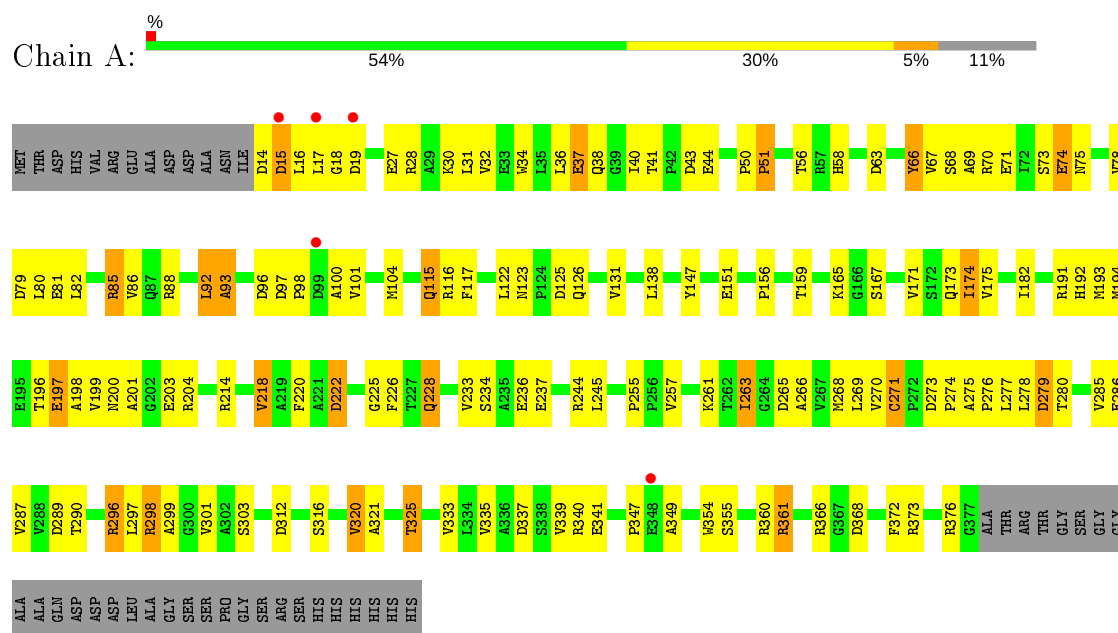


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Hypothetical protein Rv1264/MT1302



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.11Å 114.11Å 151.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 3.30 24.85 – 3.30	Depositor EDS
% Data completeness (in resolution range)	91.8 (25.00-3.30) 91.8 (24.85-3.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.61 (at 3.30Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.235 , 0.299 0.228 , 0.295	Depositor DCC
$R_{free}$ test set	408 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, 1PE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	0/2782	0.68	0/3782

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	LEU	Peptide

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2737	0	2772	102	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	0	22	1	0
4	A	6	0	8	0	0
All	All	2764	0	2802	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLU:HG3	1:A:376:ARG:HH21	1.37	0.90
1:A:68:SER:HB2	1:A:100:ALA:O	1.72	0.89
1:A:286:GLU:CG	1:A:376:ARG:HH21	1.88	0.85
1:A:287:VAL:O	1:A:290:THR:HG22	1.78	0.84
1:A:82:LEU:HD23	1:A:115:GLN:NE2	1.96	0.81
1:A:68:SER:OG	1:A:71:GLU:HG2	1.82	0.80
1:A:17:LEU:HD21	1:A:32:VAL:HG21	1.65	0.77
1:A:82:LEU:HD23	1:A:115:GLN:HE22	1.50	0.77
1:A:275:ALA:HB3	1:A:276:PRO:HD3	1.71	0.72
1:A:316:SER:O	1:A:320:VAL:HG13	1.89	0.72
1:A:316:SER:O	1:A:320:VAL:CG1	2.37	0.72
1:A:301:VAL:HB	1:A:335:VAL:HG22	1.73	0.70
1:A:335:VAL:HG13	1:A:339:VAL:HG13	1.72	0.70
1:A:69:ALA:HB3	1:A:98:PRO:HA	1.76	0.68
1:A:14:ASP:OD1	1:A:16:LEU:HB3	1.95	0.67
1:A:257:VAL:HG23	1:A:271:CYS:HB3	1.78	0.66
1:A:68:SER:CB	1:A:100:ALA:O	2.43	0.66
1:A:70:ARG:HB2	1:A:98:PRO:HB2	1.76	0.65
1:A:279:ASP:OD1	1:A:280:THR:N	2.31	0.64
1:A:220:PHE:HB2	1:A:325:THR:HG21	1.79	0.62
1:A:225:GLY:O	1:A:228:GLN:NE2	2.32	0.62
1:A:233:VAL:CG1	1:A:237:GLU:HB3	2.28	0.62
1:A:271:CYS:SG	1:A:273:ASP:O	2.58	0.61
1:A:123:ASN:HB3	1:A:126:GLN:HB2	1.83	0.59
1:A:361:ARG:NH2	1:A:366:ARG:HD2	2.19	0.58
1:A:286:GLU:CB	1:A:376:ARG:HH21	2.15	0.58
1:A:66:TYR:HA	1:A:104:MET:HA	1.86	0.58
1:A:28:ARG:HH21	1:A:51:PRO:HD3	1.67	0.58
1:A:192:HIS:O	1:A:193:MET:C	2.42	0.57
1:A:70:ARG:HA	1:A:80:LEU:HD11	1.87	0.57
1:A:196:THR:O	1:A:196:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASP:OD2	1:A:298:ARG:NE	2.34	0.55
1:A:335:VAL:HG11	1:A:354:TRP:HZ3	1.72	0.55
1:A:321:ALA:O	1:A:325:THR:HG22	2.05	0.55
1:A:56:THR:CG2	1:A:171:VAL:HG21	2.36	0.55
1:A:123:ASN:OD1	1:A:125:ASP:HB2	2.05	0.55
1:A:174:ILE:HD11	3:A:409:1PE:H241	1.89	0.55
1:A:115:GLN:HE21	1:A:115:GLN:HA	1.72	0.54
1:A:233:VAL:CG1	1:A:237:GLU:CB	2.85	0.54
1:A:44:GLU:OE2	1:A:58:HIS:NE2	2.40	0.54
1:A:28:ARG:NH2	1:A:51:PRO:HD3	2.22	0.54
1:A:286:GLU:HG3	1:A:376:ARG:NH2	2.16	0.54
1:A:70:ARG:HA	1:A:80:LEU:CD1	2.38	0.53
1:A:200:ASN:CG	1:A:201:ALA:H	2.11	0.53
1:A:71:GLU:O	1:A:75:ASN:ND2	2.27	0.53
1:A:335:VAL:HG13	1:A:339:VAL:CG1	2.37	0.53
1:A:78:VAL:HG23	1:A:115:GLN:HB2	1.91	0.52
1:A:275:ALA:HB3	1:A:276:PRO:CD	2.37	0.52
1:A:335:VAL:HG11	1:A:354:TRP:CZ3	2.46	0.51
1:A:34:TRP:O	1:A:38:GLN:HG2	2.11	0.50
1:A:79:ASP:OD1	1:A:80:LEU:N	2.45	0.50
1:A:200:ASN:OD1	1:A:204:ARG:NH2	2.44	0.50
1:A:81:GLU:O	1:A:85:ARG:HG2	2.12	0.50
1:A:86:VAL:HB	1:A:131:VAL:HG11	1.95	0.49
1:A:263:ILE:HG13	1:A:266:ALA:HB3	1.93	0.49
1:A:261:LYS:NZ	1:A:312:ASP:OD1	2.45	0.48
1:A:56:THR:HG21	1:A:171:VAL:HG21	1.96	0.48
1:A:361:ARG:HD2	1:A:368:ASP:HB3	1.96	0.48
1:A:220:PHE:CE2	1:A:268:MET:HG3	2.49	0.48
1:A:218:VAL:HG23	1:A:270:VAL:HG22	1.95	0.47
1:A:316:SER:O	1:A:320:VAL:HG12	2.12	0.47
1:A:67:VAL:HG12	1:A:68:SER:N	2.29	0.47
1:A:117:PHE:O	1:A:122:LEU:HB2	2.15	0.47
1:A:78:VAL:HG23	1:A:115:GLN:NE2	2.30	0.47
1:A:203:GLU:OE1	1:A:214:ARG:NH1	2.47	0.47
1:A:299:ALA:HB3	1:A:333:VAL:HG22	1.96	0.46
1:A:337:ASP:OD1	1:A:340:ARG:NE	2.47	0.46
1:A:361:ARG:HH22	1:A:366:ARG:HD2	1.81	0.45
1:A:167:SER:O	1:A:171:VAL:HG23	2.16	0.45
1:A:17:LEU:CD2	1:A:32:VAL:HG21	2.43	0.45
1:A:82:LEU:CD2	1:A:115:GLN:HE22	2.26	0.45
1:A:263:ILE:O	1:A:263:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLU:HB3	1:A:376:ARG:NH2	2.32	0.45
1:A:138:LEU:HD21	1:A:182:ILE:HD11	1.98	0.44
1:A:285:VAL:HA	1:A:297:LEU:HD12	1.98	0.44
1:A:274:PRO:O	1:A:275:ALA:C	2.56	0.44
1:A:296:ARG:HG3	1:A:296:ARG:H	1.58	0.44
1:A:101:VAL:O	1:A:101:VAL:HG12	2.17	0.44
1:A:66:TYR:CD1	1:A:66:TYR:N	2.86	0.44
1:A:67:VAL:CG1	1:A:68:SER:N	2.79	0.44
1:A:197:GLU:HG2	1:A:198:ALA:N	2.33	0.44
1:A:96:ASP:OD1	1:A:96:ASP:N	2.51	0.44
1:A:199:VAL:HG13	1:A:203:GLU:HB2	2.00	0.44
1:A:37:GLU:HA	1:A:37:GLU:OE1	2.18	0.44
1:A:171:VAL:HG12	1:A:175:VAL:HG23	2.00	0.43
1:A:279:ASP:OD1	1:A:279:ASP:C	2.56	0.43
1:A:92:LEU:HB3	1:A:93:ALA:H	1.57	0.43
1:A:199:VAL:HG13	1:A:203:GLU:CB	2.49	0.43
1:A:81:GLU:HA	1:A:81:GLU:OE2	2.19	0.42
1:A:303:SER:OG	1:A:339:VAL:HB	2.19	0.42
1:A:277:LEU:HD23	1:A:278:LEU:N	2.34	0.42
1:A:340:ARG:HD3	1:A:372:PHE:CZ	2.54	0.42
1:A:27:GLU:HA	1:A:27:GLU:OE2	2.19	0.42
1:A:56:THR:HG23	1:A:171:VAL:HG21	2.02	0.41
1:A:200:ASN:OD1	1:A:201:ALA:N	2.53	0.41
1:A:70:ARG:O	1:A:73:SER:HB3	2.20	0.41
1:A:263:ILE:CG1	1:A:263:ILE:O	2.68	0.41
1:A:74:GLU:H	1:A:74:GLU:HG2	1.63	0.41
1:A:36:LEU:HD23	1:A:40:ILE:O	2.19	0.41
1:A:50:PRO:HA	1:A:51:PRO:HD3	1.91	0.41
1:A:171:VAL:C	1:A:173:GLN:H	2.24	0.41
1:A:233:VAL:HG12	1:A:234:SER:N	2.35	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	362/407 (89%)	311 (86%)	41 (11%)	10 (3%)	5	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	93	ALA
1	A	156	PRO
1	A	226	PHE
1	A	347	PRO
1	A	349	ALA
1	A	15	ASP
1	A	18	GLY
1	A	255	PRO
1	A	51	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/312 (90%)	237 (85%)	43 (15%)	2	12

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	30	LYS
1	A	31	LEU
1	A	37	GLU
1	A	41	THR
1	A	43	ASP
1	A	63	ASP
1	A	66	TYR
1	A	74	GLU

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Mol	Chain	Res	Type
1	A	85	ARG
1	A	88	ARG
1	A	97	ASP
1	A	115	GLN
1	A	116	ARG
1	A	147	TYR
1	A	151	GLU
1	A	159	THR
1	A	165	LYS
1	A	174	ILE
1	A	191	ARG
1	A	194	MET
1	A	197	GLU
1	A	218	VAL
1	A	222	ASP
1	A	228	GLN
1	A	236	GLU
1	A	244	ARG
1	A	245	LEU
1	A	263	ILE
1	A	265	ASP
1	A	269	LEU
1	A	271	CYS
1	A	279	ASP
1	A	289	ASP
1	A	296	ARG
1	A	298	ARG
1	A	320	VAL
1	A	325	THR
1	A	341	GLU
1	A	355	SER
1	A	360	ARG
1	A	361	ARG
1	A	373	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	126	GLN
1	A	183	GLN
1	A	189	GLN

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Mol	Chain	Res	Type
1	A	192	HIS
1	A	293	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	408	-	4,4,4	0.38	0	6,6,6	0.35	0
3	1PE	A	409	-	15,15,15	0.85	0	14,14,14	0.47	0
4	GOL	A	410	-	5,5,5	0.36	0	5,5,5	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	A	409	-	-	4/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	410	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	410	GOL	O1-C1-C2-C3
3	A	409	1PE	OH5-C14-C24-OH4
3	A	409	1PE	OH6-C15-C25-OH5
4	A	410	GOL	C1-C2-C3-O3
4	A	410	GOL	O1-C1-C2-O2
4	A	410	GOL	O2-C2-C3-O3
3	A	409	1PE	OH7-C16-C26-OH6
3	A	409	1PE	OH4-C13-C23-OH3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	409	1PE	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	364/407 (89%)	-0.18	5 (1%) 75 75	45, 53, 61, 68	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	19	ASP	2.4
1	A	15	ASP	2.4
1	A	99	ASP	2.3
1	A	348	GLU	2.2
1	A	17	LEU	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	410	6/6	0.87	0.28	57,58,62,67	0
2	SO4	A	408	5/5	0.90	0.32	67,67,68,69	0
3	1PE	A	409	16/16	0.91	0.29	51,55,65,65	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.